Electronic States of High T_c Oxide Superconductors(Abstracts of Doctral Dissertations)

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Masahide SASAKI

Institute for Materials Reseach

Abstract

Oxide superconductors containing CuO_2 planes exhibit high transition temperature (T_c) (40~120 K). The experimental data accumulated so far indicate that the electronic state on the CuO_2 plane is responsible not only for the superconductivity but also for various anormalies in the normal state, such as T linear dc resistivity, constant continuum of electronic Raman scattering intensity and so on. Nature of the electronic state on the carrier doped CuO_2 plane is one of the central issues in study of high T_c oxide superconductors.

The characteristic feature of those cuprate oxides is in the fact that one can easily change phases of the system from an insulator to a good metal by a small amount of carrier doping. The superconductivity appears only in a restricted metallic region close to the insulator phase. The first step to elusidate the mechanism of high T_c superconductivity may be to clarify the nature of the electronic state realized in an intermediate region between the insulator and the conventional metal. The effective theory for this region has not been established yet. The purpose of this thesis is to clarify the simple physical picture for the electronic states near the Fermi level (FL) of high T_c cuprate superconductors and establish a theoretical frame work to describe it.

Several experimental studies such as photoemission, X-ray absorption spectroscopy (XAS), electron energy loss spectroscopy (EELS), infrared spectroscopy and so on reveal that spectral distributions change from the insulating-gap structure to the lower-energy one with a rapid transfer of spectral intensity by small amount of doping. In this thesis, the electronic state of CuO_2 plane is studied by asking what the mechanism of anormalous transfer of spectral weight is and how the electronic state near the FL can be described theoretically.

We start from the p-d mixing model which contains the upper Hubbard level (UHL) (ϵ_η) of the split Cu 3d states by local Coulomb repulsion U ($U \to \infty$, bare d level $\epsilon_d \to -\infty$ and $\epsilon_\eta = \epsilon_d + U$), O 2p level and the mixing interaction (t) between them. The electronic excitation with spin σ to the UHL is expressed by the operator $\eta^\dagger_\sigma = d^\dagger_\sigma d^\dagger_{-\sigma} d_{-\sigma}$ where $d^\dagger_\sigma$ and d_σ are creation and annihilation operators of d electrons with spin σ, respectively. The excitation with spin σ to the p level is described by $p^\dagger_\sigma$. Because of the large Coulomb repulsion at Cu site ($U \to \infty$ in our model), p-d electron hopping is strongly correlated with the surrounding charge and spin states.

In this thesis, it is discussed that the electronic state developing by hole doping near the FL is not bare p electronic excitation but many-body excitation accompanying d electron spin and charge fluctuations, and the operators p_s and p_0 are introduced to describe those

composite electronic excitations associated with Cu-O bond. p_s (p_0) is composed of the d electron spin (charge) fluctuation operator and the p electron annihilation operator at the neighboring site of Cu. By treating p, η, p_s and p_0 on the equal footing, it is shown that changes of the electronic states can be interpreted as changes of weight of those modes and mixing interactions among them. As for the formulation, by introducing the notation $\psi_n = (p, \eta, p_s, p_0)_n$, the renormalization factor I and the self-energy Σ for ψ_n are identified. Then the retarded Green's functions of ψ_n are defined and their equations are derived based on the equations of motion and algebra of ψ_n. Especially, we calculate Σ by separating it into the static and dynamical parts where the former represents the renormalized levels of ψ_n and effective mixing interactions among them and the latter does the damping effects for ψ_n due to spin and charge fluctuations. The normalization factor I and the static part of Σ are expressed as expectation values of anti-commutator of operators. The calculation of spin and charge fluctuations can be performed in the same manner by using a relaxation function formalism instead of a retarded one. In this framework, coupling strength among excitation modes are calculated such that the algebra at local site are satisfied.

Based on this method, we have analyzed the electronic state of the highly correlated p-d mixing model. It is shown that rapid modification of spectral-intensity distribution by hole doping is understood as the process which p_s develops to a stable excitation near the FL from a damping mode near the top of the valence band in the insulator. In the metallic region, there exist a quasi-particle band crossing the FL which can be interpreted as the anti-bonding band due to the mixing between p and p_s. These results are qualitatively consistent with the experimental results of photoemission, EELS, and XAS.

It is also shown that these rapid changes of Fermion modes are related with the changes of spin and charge fluctuations. In the insulator, charge fluctuation has a peak of insulating-gap excitation while there is a prominant peak at zero energy in spin fluctuation. As holes are doped, the spectral weight of insulating-gap excitation decreases rapidly and transfers to the low energy region in charge fluctuation, which is consistent with the results of infrared absorption experiments. On the other hand, in spin fluctuation, the intensity of a peak at zero energy decreases and its spectrum is broadened to higher energy.

The results in this thesis indicate that the electronic states of high T_c cuprate can be understood by introducing composite electronic excitations p_s and p_0 associated with Cu-O bond and by considering the mixing among p, η, p_s and p_0. Especially, nature of the electronic states around the FL is characterized by p_s and p_0 in hole doping case.